

Computable Measures for the Entanglement of Indistinguishable Particles

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We discuss particle entanglement in systems of indistinguishable bosons and fermions, in finite Hilbert spaces, with focus on operational measures of quantum correlations. We show how to use von Neumann entropy, Negativity and entanglement witnesses in these cases, proving interesting relations. We obtain analytic expressions to quantify quantum correlations in homogeneous D-dimensional Hamiltonian models with certain symmetries.

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I. INTRODUCTION

The notion of entanglement, first noted by Einstein, Podolsky and Rosen [1], is considered one of the main features of quantum mechanics, and became a subject of great interest in the last years, due to its primordial role in Quantum Computation and Quantum Information [2–5]. Despite being widely studied in systems of distinguishable particles, less attention has been given to the case of indistinguishable ones. In this case the space of quantum states is restricted to symmetric (\mathcal{S}) or antisymmetric (\mathcal{A}) subspaces, depending on the bosonic or fermionic nature of the system.

Entanglement of indistinguishable systems is much subtler than that of distinguishable ones, and there has been distinct approaches to its treatment, resulting in different notions like *quantum correlations* [6–8], *entanglement of modes* [9], and *entanglement of particles* [10]. In Zanardi's entanglement of modes [9], as well as in Wiseman and Vaccaro's entanglement of particles, a Fock space is associated to the state space of a quantum system composed by several distinguishable modes, which allows one to employ all the tools commonly used in distinguishable quantum systems. In this work we will deal with the notion of quantum correlations [6–8], which calls for different tools.

Several notions of quantum correlations have been proposed in the literature, which agree in some respects, but differ in others. According to Eckert *et al.* [6], the pure states with no quantum correlations are those described by a single Slater determinant for fermions, or a single Slater permanent formed out of a single one particle-state in the bosonic case. Li *et al.* [8] base their analysis on the resolution of the state in a direct-sum of single-particle states. Gihardi and Marinatto [7] relate the notion of entanglement of quantum systems composed of two identical constituents to the impossibility of attributing a complete set of properties to both particles. It is important to note that these different definitions agree in the fermionic case, showing that the correlations generated by mere anti-symmetrization of the state due to indistinguishability of their particles do not constitute truly as entanglement, or equivalently, states described by a single Slater determinant (Hartree-Fock approximation), which are eigenstates of the free fermions Hamiltonian (single-particle Hamiltonian), have no quantum correlations. On the other hand, such definitions may disagree with each other in the bosonic case. Entanglement of indistinguishable fermions is far simpler than that of indistinguishable bosons. The definitions by Li *et al.* [8] and Gihardi and Marinatto [7], although distinct, result in the same set of pure bosonic states without quantum correlations, which is greater than that defined by Eckert *et al.* [6]. Interestingly, as in the fermionic case, the former set corresponds to the eigenstates of the free bosons Hamiltonian, which is expected not to possess quantum correlations.

Once one has opted for a certain notion of entanglement, the next step is to devise a method to calculate it. There are some interesting operational quantum correlation measures like the Slater concurrence [6] for two fermions/bosons of dimension $\mathcal{A}(\mathcal{H}^4 \otimes \mathcal{H}^4)/\mathcal{S}(\mathcal{H}^2 \otimes \mathcal{H}^2)$; the von Neumann entropy of the single-particle reduced state for pure states of two particles [8, 11]; the linear entropy of the single-particle reduced state of N-fermion pure states [12]. In a previous work [13], we have shown how to calculate optimal entanglement witnesses for indistinguishable fermions, and introduced a new operational measure. With our witnesses we can calculate the generalized robustness of entanglement for systems with arbitrary number of fermions, with single-particle Hilbert space of arbitrary dimension. Interestingly, in the case of two fermions with a four-dimensional single-particle Hilbert space, the generalized robustness coincides with the Slater concurrence. All these measures have limitations, either conceptual or computational, and should be considered

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complementary. The quantification of quantum correlations for general states, fermionic or bosonic, remains an open problem.

In this work, as a natural extension of [13], we will show how to calculate entanglement witnesses for the bosonic case, but they will not be optimal due to some subtleties of the uncorrelated bosonic states. We will show that functions of the purity of the single-particle reduced state quantify quantum correlations for pure states, with the caveat that for some special known values, the quantifier is inconclusive for bosons. This extends previous results by Paskauskas *et. al* [11] and Plastino *et. al* [12]. We will also see that a simple shift in the well known negativity ($Neg(\rho) = \|\rho^{T_i}\|_1 - \text{constant}$) [14] results in a quantifier of quantum correlations in bosons and fermions. Finally, in the context of entanglement in many-body systems [5, 15, 16], we will analyze homogeneous D-dimensional Hamiltonian models with certain symmetries, by means of the von Neumann entropy of the single-particle reduced state.

This paper is organized as follows. In Sec.II we consider quantum correlations in fermionic states, showing how the purity of the single-particle reduced state can be used as a measure for pure states, and the Negativity for the general case. In Sec.III the same analysis is made for bosons. In Sec.IV we discuss entanglement witnesses in bosonic systems. In Sec.V we make some remarks about the different measures of quantum correlations, and discuss how they compare for pure states in the smallest dimension single-particle Hilbert space, proving some relations. In Sec.VI we show how to calculate quantum correlations in certain homogeneous D-dimensional Hamiltonian models. In the Appendix, we prove the expressions for the Negativity of bosons and fermions. We conclude in Sec.VII.

II. FERMIONS

Systems of indistinguishable particles have a more concise description in the second quantization formalism. Therefore we introduce operators with the following anti-commutation relations:

$$\{f_i^\dagger, f_j^\dagger\} = \{f_i, f_j\} = 0, \quad \{f_i, f_j^\dagger\} = \delta_{ij}. \quad (1)$$

f_i^\dagger and f_i are the fermionic creation and annihilation operators, respectively, such that their application on the vacuum state ($|0\rangle$) creates/annihilates a fermion in state “i”. The vacuum state is defined such that $f_i|0\rangle = 0$.

As stated in the Introduction, the different definitions of quantum correlations agree with each other in the fermionic case, in the sense that the set of states without quantum correlations can be defined as follows.

Fermionic state without quantum correlations: A fermionic state $\sigma \in \mathcal{B}(\mathcal{H}_1^d \otimes \dots \otimes \mathcal{H}_N^d)$ has no quantum correlations if it can be decomposed as a convex combination of Slater determinants, namely,

$$\sigma = \sum_i p_i a_1^{i\dagger} \dots a_N^{i\dagger} |0\rangle \langle 0| a_N^i \dots a_1^i, \quad \sum_i p_i = 1, \quad (2)$$

where $a_k^{i\dagger} = \sum_{l=1}^d u_{kl}^i f_l^\dagger$ ($\{a_k^{i\dagger}\}$ is a set of orthonormal operators in the index k), U^i is a unitary matrix of dimension dN , and $\{f_l^\dagger\}$ is an orthonormal basis of fermionic creation operators for the space of a single fermion (\mathcal{H}^d). Note that uncorrelated pure states are single Slater determinants. The single-particle reduced states ($\sigma_{r(s_{l_1})}$) of a single Slater determinant have a particularly interesting form, and stand for the pure states in the “N-representable” reduced space (single-particle reduced space respective to the antisymmetric space of N fermions) [17].

Single-particle reduced fermionic state without quantum correlations: Given a pure fermionic state without quantum correlations, *i.e.* a single Slater determinant, $|\psi\rangle = a_{\phi_1}^\dagger a_{\phi_2}^\dagger \dots a_{\phi_N}^\dagger |0\rangle$, where $\{a_{\phi_i}^\dagger\}$ are orthonormal, we have the equivalence:

$$\sigma_{r(s_{l_1})} \equiv \frac{1}{N} \sum_{i=1}^N a_{\phi_i}^\dagger |0\rangle \langle 0| a_{\phi_i} \iff |\psi\rangle = a_{\phi_1}^\dagger a_{\phi_2}^\dagger \dots a_{\phi_N}^\dagger |0\rangle, \quad (3)$$

where $\sigma_{r(s_{l_1})} = Tr_1 \dots Tr_{N-1}(|\psi\rangle \langle \psi|)$ is the single-particle reduced state (Tr_i is the partial trace over particle i). Therefore, if σ is a mixed uncorrelated state, its single-particle reduced state in the “N-representable” reduced space is:

$$\sigma_r \equiv Tr_1 \dots Tr_{N-1}(\sigma) = \sum_i p_i \sigma_{r(s_{l_1})}^i. \quad (4)$$

Now, aware of Eq.3, it is straightforward to conclude that shifted positive semidefinite functions of the purity of the single-particle reduced state can be used to measure the quantum correlation of a pure fermionic state, a result similar

to that obtained by Plastino *et al.* [12] or Paskauskas *et al.* [11]. Using, for example, the von Neumann entropy ($S(\rho) = \text{Tr}(-\rho \log \rho)$), we see that $S(\rho_r = \text{Tr}_1 \dots \text{Tr}_{N-1}(|\psi\rangle\langle\psi|)) \geq S(\sigma_{r_{(sl_1)}}) = \log N$, and thus a measure “ E ” for the quantum correlations of a pure fermionic state can be defined by a *shifted von Neuman entropy of the single-particle reduced state*.

Shifted von Neuman entropy of entanglement for pure states:

$$E(|\psi\rangle\langle\psi|) = S(\rho_r) - \log N. \quad (5)$$

The case of pure states is easy due to the unique form of the uncorrelated single-particle reduced states (Eq.3), which is no longer the case for mixed states (Eq.4). Though not obvious, but straightforward to prove as we show in the Appendix, we can measure the quantum correlations of mixed fermionic states by the following *shifted Negativity*.

Shifted Negativity:

$$\text{Neg}(\rho) = \begin{cases} \|\rho^{T_i}\|_1 - N & \text{if } \|\rho^{T_i}\|_1 > N, \\ 0 & \text{otherwise,} \end{cases} \quad (6)$$

where T_i is the partial transpose over the i -th particle, and $\|\cdot\|_1$ is the trace-norm. If ρ is a single Slater determinant, its trace-norm is N , and it is smaller in the case of a uncorrelated mixed state, as shown in the Appendix. Note, however, that we do not know if there are correlated fermionic states whose Negativity is null.

III. BOSONS

As in the previous section, we introduce operators to describe the bosonic system in the second quantization formalism. The operators satisfy the usual commutation relations:

$$[b_i^\dagger, b_j^\dagger] = [b_i, b_j] = 0, \quad [b_i, b_j^\dagger] = \delta_{ij}, \quad (7)$$

where b_i^\dagger and b_i are the bosonic creation and annihilation operators, respectively, such that their application on the vacuum state ($|0\rangle$) creates/annihilates a boson in state “ i ”. The vacuum state is defined such that $b_i |0\rangle = 0$.

As stated in the Introduction, the different notions of quantum correlations in bosons diverge from each other, resulting in two distinct sets of uncorrelated states.

Bosonic pure state with no quantum correlations: A bosonic pure state $|\psi\rangle \in \mathcal{S}(\mathcal{H}_1^d \otimes \dots \otimes \mathcal{H}_N^d)$, without quantum correlations, can be written as:

$$\text{Definition 1.} \quad |\psi\rangle = \prod_{i=1}^{N_o} \frac{(b_{\phi_i}^\dagger)^{n_{\phi_i}} |0\rangle}{\sqrt{(n_{\phi_i}!)}} \quad (8)$$

$$\text{Definition 2.} \quad |\psi\rangle = \frac{1}{\sqrt{N!}} (b_\phi^\dagger)^N |0\rangle, \quad (9)$$

where $b_{\phi_i}^\dagger = \sum_{k=1}^d u_{ik} b_k^\dagger$ ($\{b_{\phi_i}^\dagger\}$ is a set of orthonormal operators in the index i), U is a unitary matrix of dimension dN_o , N_o is the number of distinct occupied states, and n_{ϕ_i} is the number of bosons in the state ϕ_i . Uncorrelated mixed states are those that can be written as convex combinations of uncorrelated pure states. We clearly see that the set of states without quantum correlations according to Definition 1 includes the set derived from Definition 2, since the later is a particular case of the former, with $N_o = 1$.

Definition 2 mirrors the case of distinguishable particles. Therefore one can use the entropy of the one-particle reduced state ($S(\rho_r)$) and the usual Negativity ($\|\rho^{T_i}\|_1 - 1$) to quantify the correlations.

The problem is delicate for the Definition 1, for the equivalence between pure states without *quantum correlations* and the single-particle reduced states is no longer uniquely defined by the analogous of Eq.3. The *shifted Negativity* given by Eq.6 is still valid, but now we do know that there are correlated states with $\|\rho^{T_i}\|_1 < N$. The entropy of the one-particle reduced state gives information about the quantum correlations, but as a quantifier it must be better understood. We know that a uncorrelated bosonic pure state, according to Eq.(8), has the following one-particle reduced state:

$$\begin{aligned} \sigma_r(\phi_i, \phi_j) &= \frac{1}{N} \text{Tr}(b_{\phi_j}^\dagger b_{\phi_i} |\psi\rangle\langle\psi|) = \begin{cases} \frac{1}{N} n_{\phi_i}, & \text{if } \phi_i = \phi_j \\ 0, & \text{otherwise,} \end{cases} \\ \sigma_r &= \frac{1}{N} \sum_{i=1}^{N_o} n_{\phi_i} b_{\phi_i}^\dagger |0\rangle\langle 0| b_{\phi_i}. \end{aligned} \quad (10)$$

$\sigma_r(\phi_i, \phi_j)$ is a matrix element of σ_r . The entropy of the one-particle reduced state assumes the special values:

$$S(\sigma_r) = - \sum_{i=1}^{N_o} \left(\frac{n_{\phi_i}}{N} \right) \log \left(\frac{n_{\phi_i}}{N} \right). \quad (11)$$

Note that $0 \leq S(\sigma_r) \leq \log N$, and therefore when $S(\rho_r) > \log N$, the pure state ρ is *quantum correlated*. The pure state is also *quantum correlated* if $S(\rho_r)$ is not one of the values given by Eq.11. Take for example the case of two bosons: we have either $N_o = 1, n_{\phi_i} = 2$ and thus $S(\sigma_r) = 0$, or $N_o = 2, n_{\phi_i} = 1$ and $S(\sigma_r) = \log 2$. Given an arbitrary pure state ρ of two bosons, if $S(\rho_r) = 0$ we can say with certainty that the state has no quantum correlations, but if $S(\rho_r) = \log 2$ we cannot conclude anything, for either a state with no quantum correlations, e.g. $|\psi\rangle = b_{\phi_i}^\dagger b_{\phi_j}^\dagger |0\rangle$, or a correlated one, e.g. $|\psi\rangle = \frac{1}{\sqrt{3}}(c_i b_{\phi_i}^\dagger b_{\phi_i}^\dagger + c_j b_{\phi_j}^\dagger b_{\phi_j}^\dagger + c_k b_{\phi_k}^\dagger b_{\phi_k}^\dagger) |0\rangle$, with $c_{i,j,k} \in \mathcal{R}$, and $S(\rho_r) \in (0, \log 3]$, could have the same von Neumann entropy for the one-particle reduced state.

IV. WITNESSED ENTANGLEMENT

In this section we present a bosonic entanglement witness. In one hand it is analogous to the fermionic entanglement witness we have introduced in a previous work [13], but on the other hand it is not optimal, due to the complicated structure of the uncorrelated bosonic states.

A Hermitian operator W is an entanglement witness for a given entangled quantum state ρ [18], if its expectation value is negative for the particular entangled quantum state ($\text{Tr}(W\rho) < 0$), while it is non-negative on the set of non-entangled states \mathcal{S} ($\forall \sigma \in \mathcal{S}, \text{Tr}(W\sigma) \geq 0$). We say that W_{opt} is the optimal entanglement witnesses (OEW) for ρ , if

$$\text{Tr}(W_{opt}\rho) = \min_{W \in \mathcal{M}} \text{Tr}(W\rho), \quad (12)$$

where \mathcal{M} represents a compact subset of the set of entanglement witnesses \mathcal{W} . With OEWs we can quantify entanglement ($E(\rho)$) by means of an appropriate choice of the set \mathcal{M} [19]:

$$E(\rho) = \max(0, - \min_{W \in \mathcal{M}} \text{Tr}(W\rho)). \quad (13)$$

In the fermionic case [13], restricting the witness operators to the antisymmetric space $\{W = \mathcal{A}W\mathcal{A}^\dagger\}$, the constraint $\{W \leq \mathcal{A}\}$ defines the Fermionic Generalized Robustness ($R_g^{\mathcal{F}}$); while the constraint $\{\text{Tr}(W) = D_a\}$, where D_a is the antisymmetric N-particle Hilbert space dimension, defines the Fermionic Random Robustness ($R_r^{\mathcal{F}}$); and the constraint $\{\text{Tr}(W) \leq 1\}$ defines the Fermionic Robustness of Entanglement ($R_e^{\mathcal{F}}$). These quantifiers correspond to the minimum value of s ($s \geq 0$), such that

$$\sigma = \frac{\rho + s\varphi}{1 + s} \quad (14)$$

is a uncorrelated state (according to Eq.2), where φ can be correlated or not in the case of $R_g^{\mathcal{F}}$, is uncorrelated in the case of $R_e^{\mathcal{F}}$, and is the maximally mixed state (\mathcal{A}/D_a) in the case of $R_r^{\mathcal{F}}$.

The method for obtaining the OEW in the fermionic case is based on semidefinite programs (SDP) [20], which can be solved efficiently with arbitrary accuracy. Now we will mimic the procedure for constructing W presented in [13], and try to obtain the Generalized Robustness for bosonic states. Consider the following SDP:

$$\begin{aligned} & \text{minimize } \text{Tr}(W\rho) \\ & \text{subject to } \left\{ \begin{array}{l} \sum_{i_{N-1}=1}^d \cdots \sum_{i_1=1}^d \sum_{j_1=1}^d \cdots \sum_{j_{N-1}=1}^d (c_{i_{N-1}}^{N-1*} \cdots c_{i_1}^{1*} c_{j_1}^1 \cdots c_{j_{N-1}}^{N-1} \times \\ W_{i_{N-1} \cdots i_1 j_1 \cdots j_{N-1}}) \geq 0, \\ \forall c_i^k \in \mathcal{C}, 1 \leq k \leq (N-1), 1 \leq i \leq d, \\ SW\mathcal{S}^\dagger = W, \\ W \leq \mathcal{S}, \end{array} \right. \quad (15) \end{aligned}$$

where d is the dimension of the single-particle Hilbert space, \mathcal{S} is the symmetrization operator, $W_{i_{N-1} \cdots i_1 j_1 \cdots j_{N-1}} = b_{i_{N-1}} \cdots b_{i_1} W b_{j_1}^\dagger \cdots b_{j_{N-1}}^\dagger \in \mathcal{B}(\mathcal{H}^d)$ is an operator acting on the space of one boson, and $\{b_i^\dagger\}$ is an orthonormal basis

of bosonic creation operators. The notation $W \leq \mathcal{S}$ means that $(\mathcal{S} - W) \geq 0$ is a positive semidefinite operator. The optimal W obtained by this program is an entanglement witness, but it cannot be optimal, as we now discuss.

For an arbitrary bosonic uncorrelated state σ , the semi-positivity condition $\text{Tr}(W\sigma) \geq 0$ is equivalent to:

$$\langle 0 | b_N b_{N-1} \cdots b_1 W b_1^\dagger \cdots b_{N-1}^\dagger b_N^\dagger | 0 \rangle \geq 0, \quad (16)$$

for all orthonormal sets of creation operators $\{b_k^\dagger\}$. This condition is taken into account in the second and third lines of Eq.15 by means of the semi-positivity of the operator $b_{N-1} \cdots b_1 W b_1^\dagger \cdots b_{N-1}^\dagger$. Therefore, the entanglement witness W will not detect bosonic correlated states of the form $b_1^\dagger \cdots b_{N-1}^\dagger \tilde{b}_N^\dagger | 0 \rangle$, where \tilde{b}_N^\dagger is not orthogonal to b_N^\dagger , a problem which does not arise in the fermionic case due to the Pauli exclusion principle. In numerical tests, we noticed that the quality of W improves with the increasing of the single-particle Hilbert space dimension.

V. MEASURES INTERRELATIONS

In this section we highlight the relationship among the measures of quantum correlations for fermionic and bosonic pure states in the smallest dimension, $\mathcal{A}(\mathcal{H}^4 \otimes \mathcal{H}^4)$ and $\mathcal{S}(\mathcal{H}^2 \otimes \mathcal{H}^2)$, respectively. While the fermionic case resembles that of distinguishable qubits, the bosonic case is more intricate, due to the structure of the uncorrelated states.

For pure states of distinguishable qubits, $\rho = |\psi\rangle\langle\psi| \in \mathcal{B}(\mathcal{H}^2 \otimes \mathcal{H}^2)$, it is well known the following equivalence for Generalized Robustness $\mathcal{R}_g(\rho)$, Robustness of Entanglement $\mathcal{R}_e(\rho)$, Random Robustness $\mathcal{R}_r(\rho)$, Wootters Concurrence $C_W(\rho)$, Negativity $Neg(\rho)$, and Entropy of Entanglement $E(\rho)$ [21–24]:

$$\mathcal{R}_g(\rho) = \mathcal{R}_e(\rho) = \frac{1}{2} \mathcal{R}_r(\rho) = C_W(\rho) = Neg(\rho) \propto E(\rho). \quad (17)$$

Recall that $E(\rho)$ is the Shannon entropy of the eigenvalues $(\lambda, 1 - \lambda)$ of the reduced one-qubit state, and $C_W = 2\sqrt{\lambda(1 - \lambda)}$.

For pure two-fermion states, $\rho = |\psi\rangle\langle\psi| \in \mathcal{B}(\mathcal{A}(\mathcal{H}^4 \otimes \mathcal{H}^4))$, we have found similar relations:

$$\mathcal{R}_g^{\mathcal{F}}(\rho) = \mathcal{R}_e^{\mathcal{F}}(\rho) = \frac{2}{3} \mathcal{R}_r^{\mathcal{F}}(\rho) = C_S^{\mathcal{F}}(\rho) = \frac{1}{2} Neg(\rho) \propto E(\rho). \quad (18)$$

Note that $Neg(\rho)$, and $E(\rho)$ are the shifted measures. The relations between Robustness and Slater concurrence were observed numerically by means of optimal entanglement witnesses [13], and now we prove them. Based on the Slater decomposition $|\psi\rangle = \sum_i z_i a_{2i-1}^\dagger a_{2i}^\dagger | 0 \rangle$, where $a_i^\dagger = \sum_k U_{ik} f_k^\dagger$, we can write the following optimal decomposition (*viz* Eq.14):

$$\sigma_{opt} = \frac{1}{1+t}(\rho + t\phi_{opt}), \quad (19)$$

$$\phi_{opt} = \frac{1}{2}(a_1^\dagger a_3^\dagger | 0 \rangle \langle 0 | a_3 a_1 + a_2^\dagger a_4^\dagger | 0 \rangle \langle 0 | a_4 a_2). \quad (20)$$

Now we show that when $t = C_S^{\mathcal{F}}(\rho)$, σ_{opt} is separable and in the border of the uncorrelated states. We know that the Slater concurrence of the state is invariant under unitary local symmetric maps Φ . We can always choose Φ so that the single particle modes $\{a_i^\dagger\}$ are mapped into the canonical modes $\{f_i^\dagger\}$ [25]. Therefore $\Phi\sigma_{opt} \rightarrow \sigma'_{opt} = \frac{1}{1+t}(|\psi'\rangle\langle\psi'| + t\phi'_{opt})$, where $|\psi'\rangle = \sum_i z_i f_{2i-1}^\dagger f_{2i}^\dagger$, and $\phi'_{opt} = \frac{1}{2}(f_1^\dagger f_3^\dagger | 0 \rangle \langle 0 | f_3 f_1 + f_2^\dagger f_4^\dagger | 0 \rangle \langle 0 | f_4 f_2)$.

The Slater concurrence of σ'_{opt} is given by $C_S^{\mathcal{F}}(\sigma'_{opt}) = \max(0, \lambda_4 - \lambda_3 - \lambda_2 - \lambda_1)$, where $\{\lambda_i\}_{i=1}^4$ are the eigenvalues, in non-decreasing order, of the matrix $\sqrt{\sigma'_{opt} \tilde{\sigma}'_{opt}}$, with $\tilde{\sigma}'_{opt} = (\mathcal{K}\mathcal{U}_{ph})\sigma'_{opt}(\mathcal{K}\mathcal{U}_{ph})^\dagger$, being \mathcal{K} the complex conjugation operator, and \mathcal{U}_{ph} the particle-hole transformation. Consider the following matrix:

$$\sqrt{\sigma'_{opt} \tilde{\sigma}'_{opt}} = \sqrt{\frac{1}{(1+t)^2}(\rho' \tilde{\rho}' + t(\rho' \tilde{\phi}'_{opt} + \phi'_{opt} \tilde{\rho}') + t^2 \phi'_{opt} \tilde{\phi}'_{opt})}. \quad (21)$$

Note that “ $\sigma'_{opt}, \rho', \phi'_{opt}$ ” and their dual are all real matrices. With the aid of Eqs.19 and 20, it is easy to see that $\rho' \tilde{\phi}'_{opt} = \phi'_{opt} \tilde{\rho}' = 0$, $\phi'_{opt} \tilde{\phi}'_{opt} = \frac{1}{2} \phi'_{opt}$, and that $\rho' \tilde{\rho}'$ is orthogonal to $\phi'_{opt} \tilde{\phi}'_{opt}$. Thus Eq.21 reduces to:

$$\sqrt{\sigma'_{opt} \tilde{\sigma}'_{opt}} = \frac{1}{(1+t)}(\sqrt{\rho' \tilde{\rho}'} + \frac{t}{\sqrt{2}} \sqrt{\phi'_{opt}}). \quad (22)$$

The eigenvalues of $\sqrt{\rho' \tilde{\rho}'}$ are easily obtained by means of its Slater decomposition, and the only non null eigenvalue is given by $C_S^{\mathcal{F}}(\rho')$. $\sqrt{\phi'_{opt}}$ has just two non null eigenvalues, which are equal, given by $\frac{1}{\sqrt{2}}$ (*viz.* Eq.20). Therefore the eigenvalues of the Eq.21 are “ $\frac{1}{(1+t)}(C_S^{\mathcal{F}}(\rho'), \frac{t}{2}, \frac{t}{2}, 0)$ ”, and according to the definition of the Slater concurrence follows directly that $C_S^{\mathcal{F}}(\sigma'_{opt}) = 0$ if and only if $t \geq C_S^{\mathcal{F}}(\rho')$.

We end this section by considering pure two-boson states, $\rho = |\psi\rangle\langle\psi| \in \mathcal{B}(\mathcal{S}(\mathcal{H}^2 \otimes \mathcal{H}^2))$. We have the following relations, which can be easily verified:

$$C_S^{\mathcal{B}}(\rho) = Neg(\rho)_{def.2} \propto E(\rho)_{def.2} \quad (23)$$

In considering the measures corresponding to definition 1 of uncorrelated states (Eq.8), we see that they are related differently, since the Negativity will always be zero for such states ($\|\rho^{T_i}\|_1 \leq 2$). This is due the use of the upper limit in Eq.42 (*viz.* Appendix). We could however, instead of using this upper limit, obtain analytically the values of $\|\rho^{T_i}\|_1$ corresponding to the uncorrelated pure states, which would be equal to $\|\rho^{T_i}\|_1 = 1$ or 2, and perform a similar analysis to that made for the $S(\rho_r)_{def.1}$ in Eq.11. Thus it would be possible to relate the Negativity and the Entropy of Entanglement according to definition 1. We see therefore that the relations between the distinct measures are similar to the distinguishable case when we consider the definition 2 (Eq.9) of quantum correlations, possessing some discrepancies when we consider the definition 1.

VI. HOMOGENEOUS D-DIMENSIONAL HAMILTONIAN

In this section we see how to use the von Neumann entropy to quantify the quantum correlations in homogeneous D-dimensional Hamiltonian models, with the following properties: (1) the eigenstates are non-degenerate, and (2) the Hamiltonian commutes with the spin operator \hat{S}_z (thus \hat{S}_z and the Hamiltonian share the same eigenstates). Consider N particles of spin Σ , L^D sites (with the closure boundary condition, $L+1=1$), and an orthonormal basis $\{c_{i\sigma}^\dagger, c_{i\sigma}\}$ of creation and annihilation operators, where $\vec{i} = (i_1, \dots, i_D)$ is the spacial position vector, and $(\sigma = -\Sigma, (-\Sigma+1), \dots, (\Sigma-1), \Sigma)$ is the spin in the direction \hat{S}_z . If $\rho = |\psi\rangle\langle\psi|$ is one eigenstate according to the conditions (1) and (2), we have:

$$Tr(c_{i\sigma}^\dagger c_{\vec{i}+\vec{\delta}\sigma} \rho) = Tr(c_{k\sigma}^\dagger c_{\vec{k}+\vec{\delta}\sigma} \rho), \quad (24)$$

$$Tr(\underbrace{c_{i\sigma}^\dagger c_{j\bar{\sigma}}}_{\sigma \neq \bar{\sigma}} \rho) = 0, \quad \forall i, j, \quad (25)$$

where Eq.(24) follows from the translational invariance property of the quantum state due to the homogeneity of the Hamiltonian, while Eq.(25) follows directly from condition (2). By condition (1) of non-degeneracy and the results of the previous sections, we know that the von Neumann entropy of the single-particle reduced state can be used as a quantifier of quantum correlations. Let us calculate it.

We know that matrix elements of the reduced state are given by $\rho_r(\vec{i}\sigma, \vec{j}\bar{\sigma}) = \frac{1}{N} Tr(c_{\vec{j}\bar{\sigma}}^\dagger c_{\vec{i}\sigma} |\psi\rangle\langle\psi|)$ and, according to Eq.(25), subspaces of the reduced state with different spin “ σ ” are disjoint. We can therefore diagonalize the reduced state in these subspaces separately. Eq.(24) together with the boundary condition fix the reduced state to a circulant matrix. More precisely, for the unidimensional case ($D=1$), given the subspace with spin “ σ ” and $\{c_{i\sigma}^\dagger\}_{i=1}^L$, the reduced state is given by the following $L \times L$ matrix:

$$\rho_r^\sigma = \frac{1}{N} \begin{pmatrix} x_0 & x_1 & \cdots & x_{L-2} & x_{L-1} \\ x_{L-1} & x_0 & x_1 & & x_{L-2} \\ \vdots & x_{L-1} & x_0 & \ddots & \vdots \\ x_2 & & \ddots & \ddots & x_1 \\ x_1 & x_2 & \cdots & x_{L-1} & x_0 \end{pmatrix}, \quad (26)$$

$$x_\delta = \langle c_{(k+\delta)\sigma} c_{k\sigma}^\dagger \rangle, \quad (27)$$

$$x_0 = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = n_{k\sigma} \underbrace{=}_{eq.24} n_{i\sigma} = \frac{N_\sigma}{L}, \quad (28)$$

where $N_\sigma = \sum_{j=1}^L n_{j\sigma}$. The terms x_δ can be obtained by several methods, *e.g.* from two-point Green's function (one-particle Green's function). The eigenvalues $\{\lambda_j^\sigma\}_{j=1}^L$ of such circulant matrix are given by $\lambda_j^\sigma = \sum_{k=0}^{L-1} x_k w_j^k$, where $w_j = \exp \frac{2\pi i j}{L}$. Thus the quantum correlations of that eigenstate can be calculated from $S(\rho_r) = -\sum_{j,\sigma} \lambda_j^\sigma \log \lambda_j^\sigma$.

For higher dimensions, given the subspace of a single-particle with spin “ σ ” and $\{c_{i\sigma}^\dagger\}_{i=1}^{L^D}$, the characteristic vector of its circulant matrix (*e.g.* the first line of matrix) is given by,

[D=2]:

$$\vec{v}_c = \begin{pmatrix} [x_{00} \cdots x_{(L-1)0}] & [x_{01} \cdots x_{(L-1)1}] & \cdots \\ \cdots & [x_{0(L-1)} \cdots x_{(L-1)(L-1)}] \end{pmatrix}, \quad (29)$$

[D=3]:

$$\vec{v}_c = \begin{pmatrix} v_{z=0}^{2D} & v_{z=1}^{2D} & \cdots & v_{z=(L-1)}^{2D} \end{pmatrix}, \quad (30)$$

where $v_{z=l}^{2D} = ([x_{00l} \cdots x_{(L-1)0l}] \ [x_{01l} \cdots x_{(L-1)1l}] \ \cdots \ [x_{0(L-1)l} \cdots x_{(L-1)(L-1)l}])$ is the characteristic vector of the plane $z = l$, and $x_{\delta_x \delta_y \delta_z} = \langle c_{(lmn)\sigma}^\dagger c_{(l+\delta_x)(m+\delta_y)(n+\delta_z)\sigma} \rangle$. Thus, the eigenvalues $\{\lambda_j^\sigma\}_{j=1}^{L^D}$ of the reduced state are given by:

$$[D=2]: \lambda_j^\sigma = \sum_{l,m=0}^{L-1} x_{lm} w_j^{l+mL}, \quad (31)$$

$$[D=3]: \lambda_j^\sigma = \sum_{l,m,n=0}^{L-1} x_{lmn} w_j^{l+mL+nL^2}, \quad (32)$$

where $w_j = \exp \frac{2\pi i j}{L^D}$. If the eigenstate does not possess such properties, we can use the Negativity as a quantifier, but then we cannot provide analytic expressions.

VII. CONCLUSION

Entanglement between distinguishable particles is related to the notion of separability, *i.e.* the possibility of describing the system by a simple tensor product of individual states. In systems of indistinguishable particles, the symmetrization or antisymmetrization of the many-particle state eliminates the notion of separability, and the concept of entanglement of particles, referred in this work as *quantum correlations*, becomes subtler. If one is interested in the different modes (or configurations) the system of indistinguishable particles can assume, it is possible to use the same tools employed in systems of distinguishable particles to calculate the *entanglement of modes*. On the other hand, if one is interested in the genuine quantum correlations between particles, as discussed in the present work, one needs new tools. In this case, we have seen that quantum correlations in fermionic systems are simple, in the sense that the necessary tools are obtained by simply antisymmetrizing the distinguishable case, and one is led to the conclusion that uncorrelated fermionic systems are represented by convex combinations of Slater determinants. The bosonic case, however, does not follow straightforwardly by symmetrization of the distinguishable case. The possibility of multiple occupation implies that a many-particle state of Slater rank one in one basis can be of higher rank in another basis. This ambiguity reflects on the possibility of multiple values of the von Neumann entropy for the one-particle reduced state of a pure many-particle state. Aware of the subtleties of the bosonic case, we have proven that a *shifted* von Neumann entropy and a *shifted* Negativity can be used to quantify quantum correlations in systems of indistinguishable particles. Motivated by previous results with fermionic optimal entanglement witnesses, we have proven relations for robustness of entanglement and Slater concurrence for two-fermion systems with a four-dimensional single-particle Hilbert space, in particular showing that the Generalized Robustness and the Slater concurrence coincide for pure states. We have shown that the bosonic entanglement witness analogous to the fermionic entanglement witness is not optimal, due to the possibility of multiple-occupation in the former case. Nonetheless, numerical calculations have shown that the bosonic witness improves with the increase of the single-particle Hilbert space dimension. Finally, we have obtained analytic expressions for the calculation of quantum correlations in Homogeneous D-dimensional Hamiltonians.

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Appendix: Negativity in fermionic/bosonic states

In this appendix we calculate the trace-norm of the partial transpose of a uncorrelated fermionic/bosonic state, *i.e.* $\|\sigma^{T_i}\|_1 = \text{Tr}[(\sigma^{T_i}, \sigma^{T_i^\dagger})^{\frac{1}{2}}]$, thus proving the *shifted negativity* (Eq.6). We do so by the explicit diagonalization of the operator $(\sigma^{T_i} \sigma^{T_i^\dagger})$. Consider first the case of a fermionic/bosonic pure state $\sigma = |\psi\rangle\langle\psi|$, as given by Eq.(2)/(8), which can be rewritten as:

$$\sigma = C \sum_{\pi\pi'} \epsilon_\pi \epsilon_{\pi'} P_\pi |\phi_1 \phi_2 \dots \phi_N\rangle \langle \phi_N \dots \phi_2 \phi_1| P_{\pi'}, \quad (33)$$

with $|\psi\rangle = \sqrt{C} \sum_{\pi} \epsilon_\pi P_\pi |\phi_1 \phi_2 \dots \phi_N\rangle$, where ϕ_i, ϕ_j are either equal or orthonormal, P_π are the permutation operators, ϵ_π is the permutation parity ($\epsilon = \pm 1$ for fermions, $\epsilon = 1$ for bosons), and $C = (N!)^{-1}$ for fermions or $C = [N! \prod_{i=1}^{N_o} (n_{\phi_i}!)]^{-1}$ for bosons. From now on we omit the normalization C and introduce the following notation:

$$P_\pi |\phi_1 \dots \phi_N\rangle = |\pi(\phi_1 \dots \phi_N)\rangle = |\pi(\phi_1) \pi(\phi_2) \dots \pi(\phi_N)\rangle. \quad (34)$$

Now we make the partial transpose on the first particle explicit:

$$\sigma^{T_1} = \sum_{\pi\pi'} \epsilon_\pi \epsilon_{\pi'} |\pi'(\phi_1) \pi(\phi_2 \dots \phi_N)\rangle \langle \pi'(\phi_N \dots \phi_2) \pi(\phi_1)|; \quad (35)$$

$$(\sigma^{T_1})^\dagger = \sigma^{T_1}; \quad (36)$$

$$\begin{aligned} \sigma^{T_1} \sigma^{T_1} &= \sum_{\pi, \pi', \tilde{\pi}, \tilde{\pi}'} \epsilon_\pi \epsilon_{\pi'} \epsilon_{\tilde{\pi}} \epsilon_{\tilde{\pi}'} |\pi'(\phi_1) \pi(\phi_2 \dots \phi_N)\rangle \\ &\quad \langle \pi'(\phi_N \dots \phi_2) \pi(\phi_1) | \tilde{\pi}'(\phi_1) \tilde{\pi}(\phi_2 \dots \phi_N)\rangle \langle \tilde{\pi}'(\phi_N \dots \phi_2) \tilde{\pi}(\phi_1)|; \end{aligned} \quad (37)$$

$$\begin{aligned} \sigma^{T_1} \sigma^{T_1} &= \sum_{\pi', \tilde{\pi}} \epsilon_{\pi'} \epsilon_{\tilde{\pi}} \langle \pi'(\phi_N \dots \phi_2) | \tilde{\pi}(\phi_2 \dots \phi_N)\rangle |\pi'(\phi_1)\rangle \langle \tilde{\pi}(\phi_1)| \otimes \\ &\quad \sum_{\pi, \tilde{\pi}'} \epsilon_\pi \epsilon_{\tilde{\pi}'} \langle \pi(\phi_1) | \tilde{\pi}'(\phi_1)\rangle |\pi(\phi_2 \dots \phi_N)\rangle \langle \tilde{\pi}'(\phi_N \dots \phi_2)|. \end{aligned} \quad (38)$$

We analyze only the bosonic case, and the fermions follow by setting $N_o = N$ and $n_{\phi_i} = 1$. Consider the first line of Eq.38. As states ϕ_i are not necessarily orthogonal, and may be the same, we have contributions when the permutations $\pi', \tilde{\pi}$ are equal and in some cases even when they are different. It can be seen that there are $n_k[(N-1)!]$ permutations such that $\pi'(\phi_1) = \phi_k$, and for each of these there are $\prod_{i=1}^{N_o} (n_{\phi_i}!)$ permutations $\tilde{\pi}$ such that $\tilde{\pi}(\phi_1) = \phi_k$, resulting in non null contributions $\langle \pi'(\phi_N \dots \phi_2) | \tilde{\pi}(\phi_2 \dots \phi_N)\rangle \neq 0$. If $\tilde{\pi}(\phi_1) \neq \phi_k$ then the contribution is null $\langle \pi'(\phi_N \dots \phi_2) | \tilde{\pi}(\phi_2 \dots \phi_N)\rangle = 0$ (simply note that the set $\{\tilde{\pi}(\phi_2 \dots \phi_N)\}$ always has n_k states “ ϕ_k ”, whereas $\{\pi'(\phi_N \dots \phi_2)\}$ has only $n_k - 1$). The first line of Eq.38 thus reduces to:

$$\sum_{k=1}^{N_o} n_k [(N-1)!] \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right] |\phi_k\rangle \langle \phi_k|. \quad (39)$$

Now we analyze the second line of Eq.38. This term has non null contributions only if $\pi(\phi_1) = \tilde{\pi}'(\phi_1)$. For permutations of the type $\pi(\phi_1) = \tilde{\pi}'(\phi_1) = \phi_k$, the matrix $|\pi(\phi_2 \dots \phi_N)\rangle \langle \tilde{\pi}'(\phi_N \dots \phi_2)|$ can assume $\frac{(N-1)!}{(n_k-1)! \prod_{i=1, (i \neq k)}^{N_o} (n_{\phi_i}!)} = \frac{n_{\phi_k} (N-1)!}{\prod_{i=1}^{N_o} (n_{\phi_i}!)}$

distinct combinations from the elements of the set $\{\pi(\phi_2 \dots \phi_N)\}$. Note that there are $\prod_{i=1}^{N_o} (n_{\phi_i}!)$ permutations of type $\pi(\phi_1) = \phi_k$ generating the same “ket” $|\pi(\phi_2 \dots \phi_N)\rangle$ (or “bra” $\langle \tilde{\pi}'(\phi_N \dots \phi_2)|$). Thus we have,

$$\sum_{\pi, \tilde{\pi}'} \epsilon_{\pi} \epsilon_{\tilde{\pi}'} \langle \pi(\phi_1) | \tilde{\pi}'(\phi_1) \rangle |\pi(\phi_2 \dots \phi_N)\rangle \langle \tilde{\pi}'(\phi_N \dots \phi_2)| = \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right]^2 |\psi_k\rangle \langle \psi_k|, \quad (40)$$

where $|\psi_k\rangle = \sum_i |\pi_k^i(\phi_2 \dots \phi_N)\rangle$, being $\pi_k^i(\phi_2 \dots \phi_N)$ all the possible permutations such that $\pi_k^i(\phi_1) = \phi_k$, and $\langle \pi_k^i(\phi_2 \dots \phi_N) | \pi_k^j(\phi_2 \dots \phi_N) \rangle = \delta_{ij}$. We have then $\langle \psi_k | \psi_{k'} \rangle = \frac{n_{\phi_k} (N-1)!}{\prod_{i=1}^{N_o} (n_{\phi_i}!)}$ $\delta_{kk'}$, and finally the second line of Eq.38 is reduced to:

$$\sum_{k=1}^{N_o} \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right]^2 |\psi_k\rangle \langle \psi_k| = \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right] (N-1)! \sum_{k=1}^{N_o} n_{\phi_k} \frac{|\psi_k\rangle \langle \psi_k|}{\langle \psi_k | \psi_k \rangle}. \quad (41)$$

From Eq.(39) and Eq.(41) and remembering to reintroduce the normalization constant C, we obtain:

$$\left\| |\psi\rangle \langle \psi|^{T_A} \right\|_1 = \frac{\left(\sum_{k=1}^{N_o} \sqrt{n_{\phi_k}} \right)^2}{N} \leq N. \quad (42)$$

The last step follows by noting that $\sum_{k=1}^{N_o} n_k = N$, and thus $\sum_{k=1}^{N_o} \sqrt{n_k} \leq N$. As the trace-norm is a convex function, we can write for uncorrelated mixed states: $\left\| \sum_j p_j \sigma_j^{T_i} \right\|_1 \leq \sum_j p_j \left\| \sigma_j^{T_i} \right\|_1$, and we are done.

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